

SPACE FILLING REPRESENTATION OF OBJECT OF CRYSTALLOGRAPHIC OR BIOLOGIC INTEREST

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Abstract: It is of the utmost importance, in various fields of sciences such as cristallography or biology, to understand the spatial relationships inside the object under study.

3D solid modelisation is a much better means to give a good understanding of the shape of an object than the use of calligraphic representations with grids. It is a precious help to apprehend the structure of the object when studying macromolecules or biological cells. However computation is much too long to allow a real time animation of the image.

We have developped two different methods to draw such images; they can be classified in two different categories:

- 1 - The object is known through the knowledge of its surface. This is the case, for instance, in cristallography, where the positions and the radius of the atoms are known. It is possible to draw a realistic image and this applies to any object as long as it may be described by quadric surfaces. We have used this method to draw the contact surface of a macromolecule: the surface is mathematically described as the envelope of a ball rolling on the molecule. This method leads to better and faster representations than using the usual facets representation each time the object may be described with less quadric than facets.

- 2 - The object is a structure described as successive planes. This is the case, for instance, of biologic serial sections as observed in electron microscopy. It is possible to obtain images of good quality without the use of a powerful computer: we have implemented this software in an image workstation. This method applies to any domain where an object may be described as a set of planes, such as scanner images or Fourier maps in cristallography.

We will discuss the advantages and the limitations of these methods and show their limitations.

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